

# An exact lower energy bound for the infinite square well potential

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We give a lower bound for the energy of a quantum particle in the infinite square well. We show that the bound is exact and identify the well known element that fulfils the equality. Our approach is not direct dependent on the Schrödinger equation and illustrates an example where the wavefunction is obtained direct by energy minimization. The derivation presented can serve as an example of a variational method in an undergraduate level university course in quantum mechanics.

## INTRODUCTION

In the introductory study of quantum mechanics the three probably most basic examples to master for the student are: the infinite square well, the harmonic oscillator and the (non-relativistic) Hydrogen atom, see e.g. [1]. These can all be solved exactly from the Schrödinger equation with moderate knowledge in mathematics. Their solutions illustrate the emergence of (bound) quantized states, hence a dramatic deviation from the classical picture. The energy spectrum for these three integrable examples can also be solved by semiclassical quantization methods [2]. Remarkably all exact energies can be obtained analytically, relying on the fact that their Hamilton functions are quadratic forms (after a coordinate transformation in the Hydrogen case [3]). These simple concepts are still very important ingredients in today's research frontier in (many-body) quantum physics, see e.g. [4], [5] and [6] respectively, for a heuristic model of a Fermi gas at unitarity, too see the emergence of super-shell structures in a harmonic trap and to model quantum information processing with Rydberg atoms.

There are not so many other examples of potentials that allow for an exact analytic treatment. For example the finite square well is of great practical importance and it helps in understanding the physics of modern man made low-dimensional structures and quantum well devices. However, it can not be solved exact although many practical (some also analytic) approximations exists [7]. In the following we discuss the obviously more artificial infinite square well, while the present notes does not provide any new results, it highlights an alternative path [8], and can be used as a simple example of a variational method.

## THE INFINITE SQUARE WELL

The infinite square well potential is here defined as

$$V(x) = \begin{cases} 0 & \text{if } 0 \leq x \leq L \\ \infty & \text{else} \end{cases}, \quad (1)$$

where the wavefunctions to the potential of Eq. (1) obey

$$\psi(0) = \psi(L) = 0. \quad (2)$$

This agrees with the probability interpretation, that the particle can not be found in finite regions where  $V = \infty$ . The usual way to obtain the lowest energy (eigenvalue) is to solve the following Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi, \quad 0 \leq x \leq L. \quad (3)$$

The point of the current note, however, is to show how to accurately estimate the lowest energy  $\min(E)$  without explicit use of the Schrödinger equation or its eigenvalues.

## HEISENBERG INEQUALITY

A standard approach is to start from the Heisenberg uncertainty relation for the momentum and position [9]

$$\Delta p \Delta x \geq \frac{\hbar}{2}. \quad (4)$$

This gives an approximate bound for the groundstate energy [10] in the potential of Eq. (1), where  $\Delta x \sim L/2$

$$E = \frac{\langle \hat{p}^2 \rangle}{2m} \sim \frac{(\Delta p)^2}{2m} \geq \frac{\hbar^2}{2mL^2}. \quad (5)$$

Since the energy spectrum to Eq. (3) is

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}, \quad n = 1, 2, \dots \Rightarrow \min(E) = E_1. \quad (6)$$

The lower bound of the estimate in Eq. (5) is hence predicting the true lowest energy  $E_1$  wrong by a factor  $\pi^2$ . This is only acceptable for very crude estimates [11], such as comparing the energy of systems of different sizes  $L$  (e.g. nuclei [MeV] and atoms [eV]).

## AN EXACT INEQUALITY

We now derive a stricter lower bound of the ground-state energy to the infinite square well potential defined in Eq. (1). Let us denote the wavefunction of the ground-state with  $\psi_0$ , this should obey the boundary conditions of Eq. (2) together with the normalization condition

$$\int_0^L |\psi(x)|^2 dx = 1. \quad (7)$$

Under those subsidiary conditions the groundstate  $\psi_0$  should minimize the energy functional (here  $\hat{H} = |\hat{p}|^2/2m$ , where we use  $\hat{p} = -i\hbar d/dx$  [12] and integration by parts)

$$E(\psi) = \langle \psi | \hat{H} | \psi \rangle = \frac{\hbar^2}{2m} \int_0^L \left| \frac{d\psi(x)}{dx} \right|^2 dx. \quad (8)$$

Our main task here is to prove the following inequality

$$E(\psi) \geq \frac{\hbar^2 \pi^2}{2mL^2}, \quad (9)$$

without using the Schrödinger equation (3), which is the Euler-Lagrange equation to (8). We then find the element  $\psi_0$  which gives equality in Eq. (9). Combining Eqs. (7) and (8) we can write the inequality of Eq. (9)

$$\int_0^L \left| \frac{d\psi(x)}{dx} \right|^2 dx \geq \frac{\pi^2}{L^2} \int_0^L |\psi(x)|^2 dx. \quad (10)$$

We remark that a related inequality have been proved with geometrical methods by Wilhelm Wirtinger already in the 19th century, see e.g. [13].

## PROOF OF THE INEQUALITY

We expand  $\psi$  to an odd function  $\tilde{\psi}$  on the interval  $-L \leq x \leq L$ , hence  $\tilde{\psi}(-L) = \tilde{\psi}(L) = 0$  [Eq. (2)]. It is natural to express  $\tilde{\psi}$  as a Fourier series  $\tilde{\psi} = \sum_k a_k \phi_k$ , with  $\phi_k = \exp(\pi i k x / L) / \sqrt{2L}$ . It then follows that

$$\frac{d\tilde{\psi}}{dx} = \sum_k \frac{\pi i k}{L} a_k \phi_k, \quad (11)$$

(using that  $d\psi/dx$  is a continuous function in  $0 < x < L$ , that  $\tilde{\psi}(-L) = \tilde{\psi}(L)$  and integration by parts.) This transforms Eq. (10) into

$$\int_{-L}^L \left( \left| \sum_{k \neq 0} k a_k \phi_k \right|^2 - \left| \sum_{k \neq 0} a_k \phi_k \right|^2 \right) dx \geq 0, \quad (12)$$

since  $a_0 = \int_{-L}^L \tilde{\psi} \phi_0 dx = 0$  as  $\tilde{\psi}$  is odd. Using the orthogonality of the  $\phi_k$ 's gives

$$\sum_{k \neq 0} (k^2 - 1) |a_k|^2 \geq 0, \quad (13)$$

and hence the inequality ( $\geq$ ) is proved. The equality ( $=$ ) is seen to be fulfilled for the elements  $\psi_0$  such that  $a_{-1} = -a_1 \neq 0$  (since  $\tilde{\psi}$  is odd) and  $a_k = 0$  for all other  $k$ . Since we choose  $\psi_0$  to be positive and real, this means that the normalized wavefunction on  $0 \leq x \leq L$  which minimize the energy is

$$\psi_0(x) = e^{3\pi i/2} (\phi_1 - \phi_{-1}) = \sqrt{2/L} \sin(\pi x/L), \quad (14)$$

as desired. The groundstate momentum relation  $p = \hbar\pi/L = \sqrt{2mE}$  then also follows from Eq. (9). We finally remark that other basis can be used to prove Eq. (10) by expanding  $\psi$ , but the equality with Eq. (14) then in general have to be checked by projection.

## CONCLUSIONS

We have obtained the well known groundstate of the infinite square well analytically without directly solving the Schrödinger equation. This derivation can serve as a neat pedagogical tool in undergraduate quantum mechanics classes. It stresses the view that the shape of the wavefunction is such that the energy is minimized, which is widely used for approximations to more complicated (many-body) systems.

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